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THEORETICAL STUDIES OF SHOCK DYNAMICS IN TWO-DIMENSIONAL STRUCTURES V. MICROSCOPIC CONSTRAINTS ON SHOCK-INDUCED SIGNALS*

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ABSTRACT

Molecular dynamics calculations are presented that address the extent of microscopic detail that can be deduced from macroscopic gauge measurements of shock propagation in condensed systems. We have simulated large asymmetrically shock-loaded lattices, varying the initial temperature and the strength of shock loading. We have also introduced randomly-placed mass defects into the lattice, and we have studied the degradation of the shock front with the subsequent development of fracture and chunky spall and have compared this with the coherent microscopic spall found for perfect lattices.

I. INTRODUCTION

An extensive series of molecular dynamics calculations has been performed that addresses the question of the extent to which microscopic detail can, in fact, be deduced from macroscopic measurements of shock propagation in condensed systems. These measurements are those that would typically be taken by Manganin or electromagnetic particle-velocity gauges. In our computer studies we have simulated large asymmetrically shock-loaded lattices, varying both initial temperature and strength of shock loading. Several concentrations of randomly placed mass defects have been introduced into the lattice; the resulting degradation of the shock front, together with the development of fracture and chunky spall, has been studied and compared with the coherent microscopic spall found to occur with perfect lattice structures.

Computer molecular dynamics involves the numerical solution by computer of Newton's equations of motion for all atoms comprising the active region of the assembly. The force acting on each particle is the resultant of all interactions with other atoms in the neighborhood and is obtained as the derivative of an effective many-body potential. The initial positions and velocities of the particles represent the initial conditions of the problem.[1] Thus the coordinates and velocities of the particles are obtained as functions of time.

II. RESULTS

The present simulations were designed to study the degree to which shocks launched into the same system, but separated in both space and time, maintain their individual integrity. We also wished to determine the influence on this integrity of: (a) the presence of random thermal motion, (b) the size of the specimen, and (c) the presence of mass defects. To this end, two basic lattices were studied: one consisting of 10 columns and 65 rows of atoms and one containing the same number of rows but with 30 columns. In each system the shocks were generated by a triplet of small flying plates, well-separated vertically, initially moving to the right with the same uniform horizontal velocity, and offset to the left by different amounts. This initial situation, illustrated for the thinner lattice by the t = 0 configuration in Fig. 1,

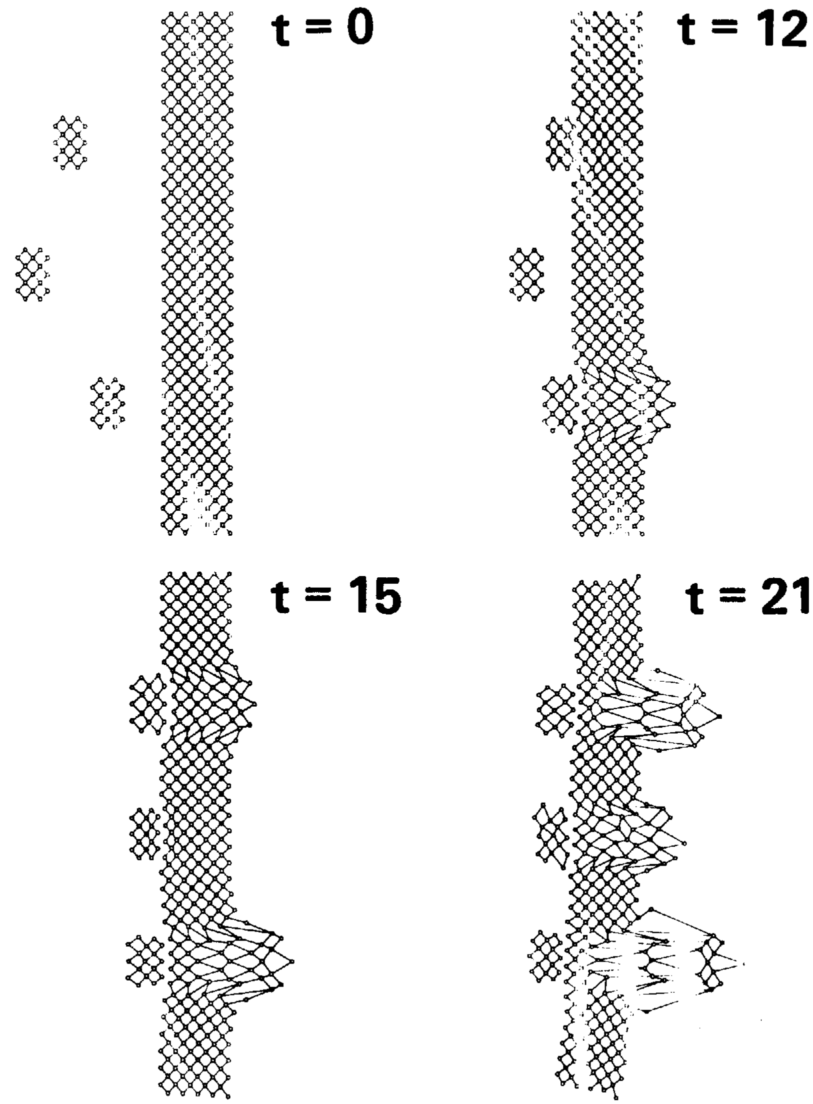

FIGURE 1.

results in the successive generation of three spatially well-separated shocks. In the present studies the bond parameters are the same for both the plates and the lattice and for both first and second neighbor bonds. Except for defects all masses are equal. (The actual parameters are those for our "model system" discussed in Ref. 2.) The initial situation is shown in Fig. 3 for the thicker lattice. Also shown on this figure are the locations where impurity atoms were introduced. In Figs. 1, 2, 4, and 5 we show sequences of configurations from the histories of seven different simulations.

In all of the present calculations carried out on perfect lattices, shock coherence and stability are clearly evident and in qualitative accord with earlier results.[2] Most importantly, in lattices without impurities the lateral transfer of energy is minimal, as shown by the development of three virtually isolated successive spalls in the initially quiescent lattices of Figs. 1 and 4 and also in the thermally highly-excited lattices shown in Fig. 2. A further measure of this lack of lateral energy transfer is the degree to which each spall event is symmetric when the lattice is initially quiescent. It can be seen from Fig. 4 that, even for the thicker lattice, this symmetry is preserved to a surprising degree. In every case a major fraction of the incoming plate energy is carried off by microscopic spall as the associated shock reaches the far surface: proportionally, the remainder of the system picks up very little energy. We also observe a very interesting demonstration of what can be referred to as a "memory effect," in that the subsequent history of the shocked system "remembers" the details of the initial loading. Thus, after multiple shock transit through the lattice and the emergency of well-separated spall from the far wall, there is a direct relationship between the pattern of ejected material and that of the initial loading.

The results obtained for shock propagation through imperfect lattices show that coupling of shock energy to defect vibrations occurs readily within the front. Furthermore, these vibrations are initially strongly localized and provide an effective mechanism for lattice disruption near the defect. The manner in which this takes place is

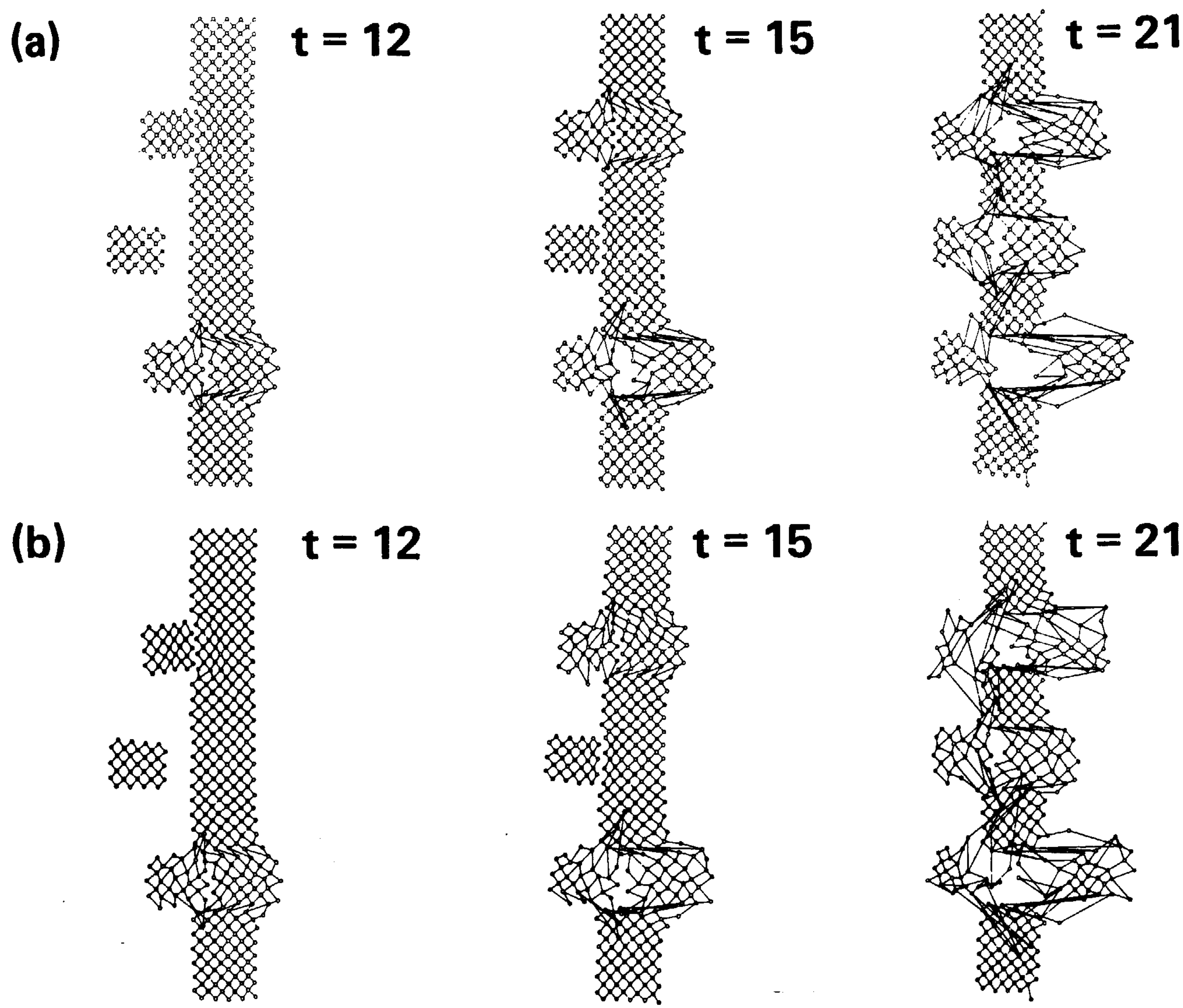

FIGURE 2.

t = 0

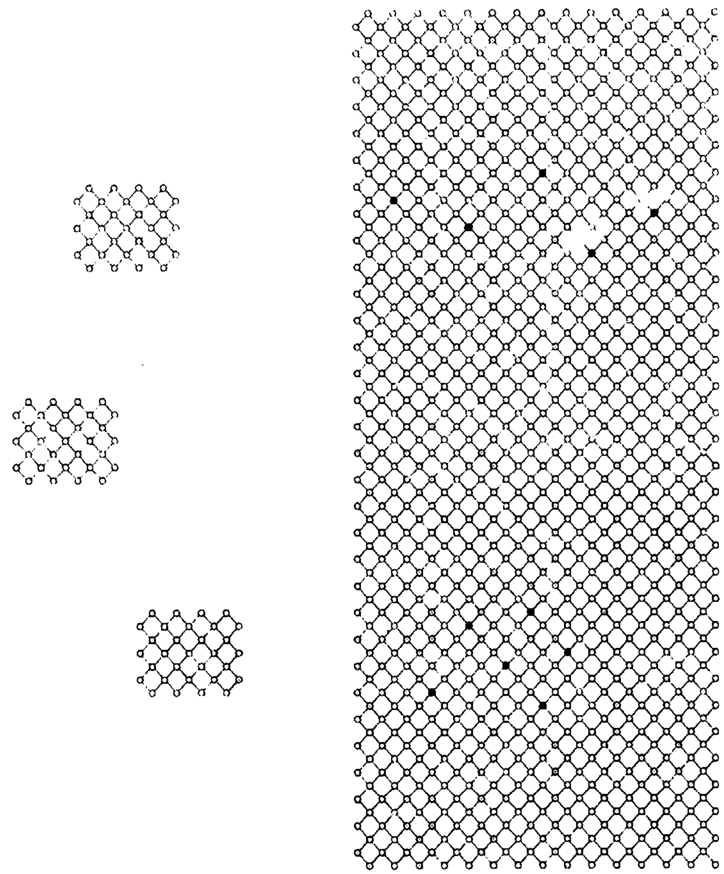

FIGURE 3.

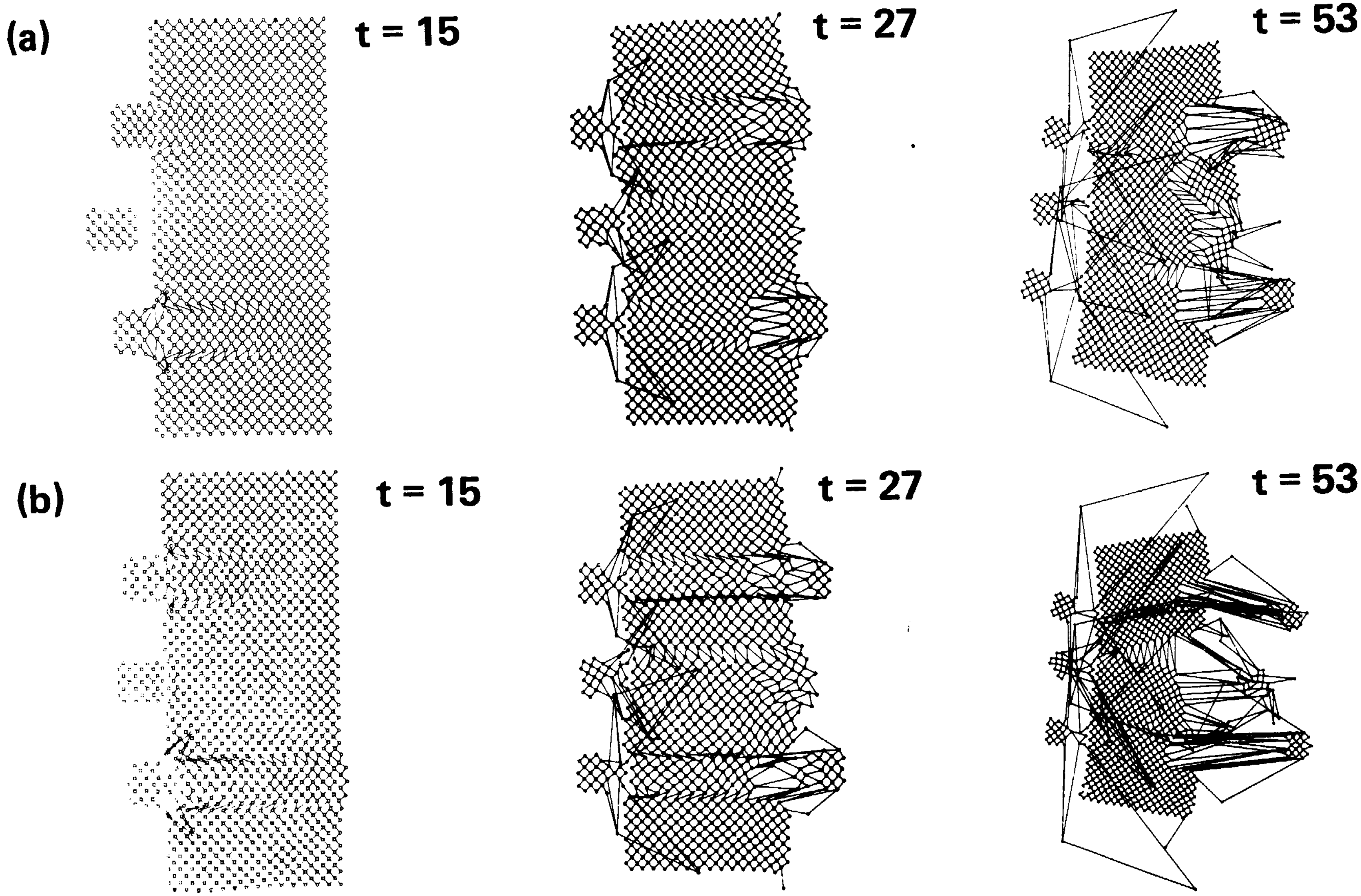

FIGURE 4.

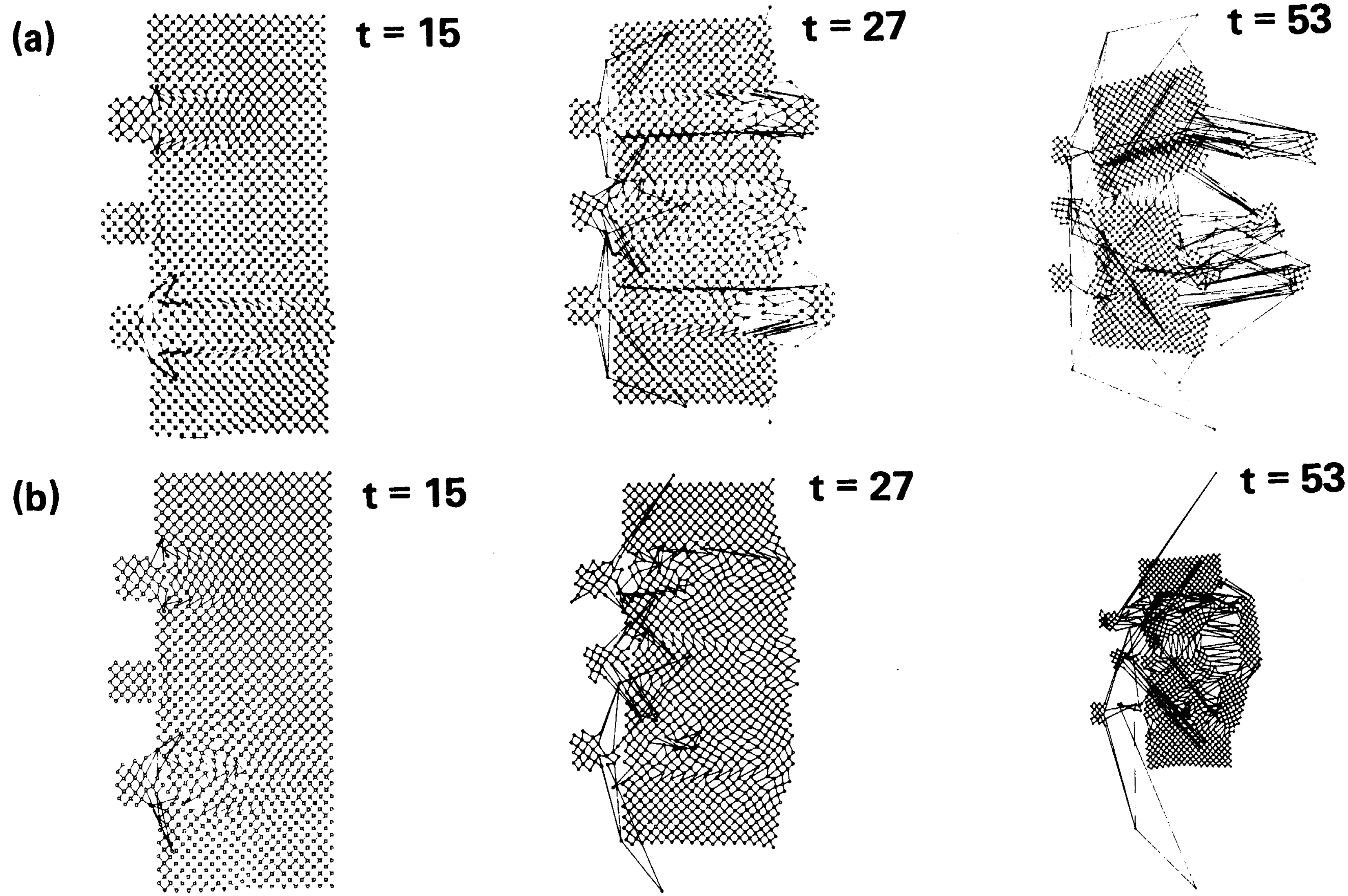

FIGURE 5.

qualitatively different for light and heavy impurities. The results shown in Fig. 5 clearly demonstrate this. Heavy impurities appear to pick up more energy from the shock front as it passes, but the resonant vibrations that develop damp out rapidly, producing widespread lattice fracture and chunky spall, nucleated where the defect concentration is highest. Light impurities tend to take up less vibrational energy, which remains essentially localized: as a result, light impurities have remarkably little effect on the shock. It is only later that we can see evidence of the considerable local distortion and damage anticipated from earlier studies.[2] Again, as expected, this damage is most marked where the impurity concentration is highest.

Finally, in Fig. 6, we show where the present studies lie on the appropriate Hugoniot plot of shock velocity versus particle velocity. This clearly demonstrates that the present shock loading is at the lower limit of those used in experimental studies. Thus, the effects that we have described in the present studies should always be present in any experimental situation, since earlier results[2] show that they are enhanced by heavier shock loading.

III. CONCLUSIONS

The present calculations show that the overall pattern of events results from a sequence of microscopic (i.e., atomic or molecular) processes occurring in picoseconds over dimensions of angstroms. It can readily be seen that for shock or detonation waves propagating in solids at 5 to 9 mm/μs, or 5 to 9 A in 10^{-13} s, and with impurities or structural irregularities no larger than 10 μ, an apparent shock rise time of 1 to 2 ns would be the shortest time obtainable. Measurements made at shorter time intervals would only be probing inhomogeneities associated with the intrinsic random defect structure of the material. Even if sample preparation could be improved to the extent that the defects or microcrystalline features in the material would be no more than 0.1 μ and even with subpicosecond instrumentation, the measured, or apparent, rise time would still be about 0.01 to 0.02 ns, i.e., about 100 times the periods associated with phenomena occurring on atomic and molecular scales.

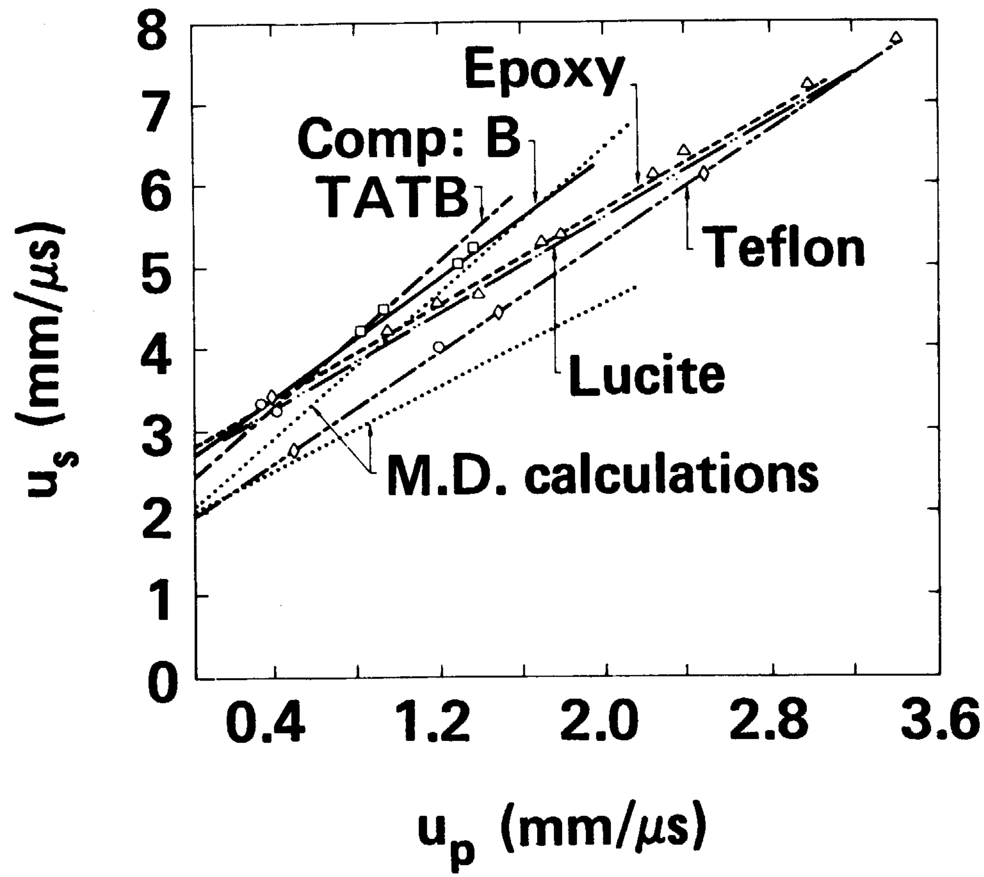
Epoxy
Comp: B
TATB
Teflon
Lucite
M.D. calculations
8
7
6
5
4
3
2
1
0
0.4
1.2
2.0
2.8
3.6
u_s (mm/μs)
u_p (mm/μs)

FIGURE 6.

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FIGURE CAPTIONS

Figure 1. Configurations of the initially quiescent 10 x 65 lattice at a sequence of times t as the shocks launched by the triplet of plates, initially moving towards the lattice at $t = 0$ with a velocity of 1.4 units, transit the lattice: at $t = 12$ the first spall is complete, at $t = 15$ the second spall is complete, and at $t = 21$ the third spalled fragment is clearly separated.

Figure 2. Configurations corresponding to those in Fig. 1 except for initial thermal motion: (a) thermal motion per bond ~5% of the dissociation energy, and (b) thermal motion per bond ~20% of the dissociation energy. For both cases the spall sequence is strikingly similar to that for the quiescent system.

Figure 3. Configuration of the 30 x 65 lattice system and associated triplet of loading plates. The sites at which mass defects can be introduced are indicated by circles.

Figure 4. Configurations of the initially quiescent triple-loaded 30 x 65 system at a sequence of times t for two different plate velocities: (a) $v = 1.2$ units and (b) $v = 1.4$ units. For both systems the first spall is about to commence at $t = 15$, and at $t = 27$ double spall is clearly apparent. At $t = 53$ we see the final state of both systems. Each shows clear double spall: in sequence (b) the central shock has produced a further spall; for sequence (a) this central spall is less definitive.

Figure 5. Configurations for two initially quiescent 30 x 65 systems containing defects: (a) light mass defects at the sites indicated in Fig. 3, and (b) heavy mass defects at the same sites. Initial plate velocities are 1.4 units. The onset of disruption of both shock and lattice is already apparent at $t = 15$ when heavy defects are present. For light defects such effects are not present.

Figure 6. Theoretical Hugoniots for two different lattice models compared with experimental data. The positions of our systems are indicated by the arrow pointing to the upper M. D. Hugoniot, corresponding to our lattice.

REFERENCES

1. B. J. Alder and T. E. Wainwright, J. Chem. Phys. 31, 459 (1959).

2. A. M. Karo and J. R. Hardy, in Proceedings of the NATO Advanced Study Institute on Fast Reactions in Energetic Systems, edited by C. Capellos and R. F. Walker (D. Reidel Publishing Co., 1981).